

# As-triazino[5,6-b]indole-3-thiol, 5-methyl-

<b>Inchi:</b>	InChI=1S/C10H8N4S/c1-14-7-5-3-2-4-6(7)8-9(14)11-10(15)13-12-8/h2-5H,1H3,(H,11,13,
<b>InchiKey:</b>	RZYGCPYYIBGBCX-UHFFFAOYSA-N
<b>Formula:</b>	C10H8N4S
<b>SMILES:</b>	Cn1c2ccccc2c2nnc(S)nc21
<b>Mol. weight [g/mol]:</b>	216.26
<b>CAS:</b>	4046-70-2

## Physical Properties

Property code	Value	Unit	Source
log10ws	-6.18		Crippen Method
logp	1.805		Crippen Method
mcvol	149.650	ml/mol	McGowan Method

## Sources

<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C4046702&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C4046702&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>

## Legend

<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume

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